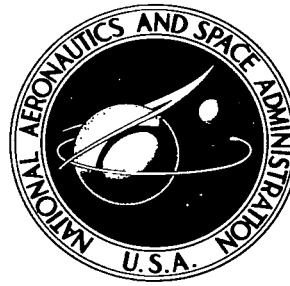


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APPROXIMATE SOLUTIONS OF RUNGE-KUTTA EQUATIONS

by Joseph S. Rosen

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By Joseph S. Rosen

George C. Marshall Space Flight Center
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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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APPROXIMATE SOLUTIONS OF THE RUNGE-KUTTA EQUATIONS

SUMMARY

In this article we are concerned with the determination of the parameters which enter the higher-order Runge-Kutta processes which are used for the numerical solution of differential equations. As the order of the process increases, the number and the complexity of the system of equations which determine the parameters in the Runge-Kutta formulation increases; also, the number of the evaluations of the function which is being integrated increases rapidly with the order. Since the latter is frequently the most time consuming computational aspect of the integration problem, approximate Runge-Kutta formulations which reduce the number of these evaluations without impairing the efficiency of the process are acceptable. Some of the techniques for obtaining these parameters—and the nature of the approximations engendered—are examined here for particular orders as these involve general aspects which persist and are as pertinent in the higher-order approximations.

THE RUNGE-KUTTA METHOD

We briefly indicate the Runge-Kutta process which leads to an algebraic system of equations whose solutions give the parameters involved.

Consider the initial value problem

$$y' = f(x, y) \qquad y(x_0) = y_0 \quad . \qquad (1)$$

We define the sequence of N quantities

$$\begin{aligned} k_1 &= hf(x_0, y_0) \\ k_2 &= hf(x_0 + \alpha_2 h, y_0 + \beta_{21} k_1) \\ k_3 &= hf(x_0 + \alpha_3 h, y_0 + \beta_{31} k_1 + \beta_{32} k_2) \\ k_4 &= hf(x_0 + \alpha_4 h, y_0 + \beta_{41} k_1 + \beta_{42} k_2 + \beta_{43} k_3) \end{aligned} \qquad (2)$$

$$k_5 = hf(x_0 + \alpha_5 h, y_0 + \beta_{51}k_1 + \beta_{52}k_2 + \beta_{53}k_3 + \beta_{54}k_4)$$

•
•
•
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$$k_N = hf\left(x_0 + \alpha_N h, y_0 + \sum_{j=1}^{n-1} \beta_{Nj} k_j\right),$$

and the linear form

$$y(x_0 + h) \approx y_0 + \sum_{i=1}^n \omega_i k_i \quad (3)$$

such that the expansion of this in powers of h agrees with the exact solution of equation (1) to a prescribed number of terms.

It is the usual practice in determining the parameters in equations (2) to expand these functions in Taylor series about the initial point (x_0, y_0) so that, to a given order, equation (3) is identical with the Taylor expansion

$$y(x_0 + h) = y_0 + hf(x_0, y_0) + \frac{h^2}{2!} f^I(x_0, y_0) + \frac{h^3}{3!} f^{II}(x_0, y_0) + \dots \quad (4)$$

which is the true solution of equation (1). Here the superscripts denote total derivatives with respect to x , which in terms of the partial derivatives increases in complexity as the order increases. On equating the respective coefficients of the partial derivative in these expansions to a given order in h , we are led to the system of equations which determine the parameters in equations (2).

Kopal [1], using the classical Taylor series expansion, derives — and gives a number of solutions for — the Runge-Kutta equations through the fourth-order. Shanks [2, 3] and Butcher [4-6], again basing their work on Taylor series expansions, show how the Runge-Kutta formulations may be made for higher orders. The writer¹, in a basically new approach to this classic Runge-Kutta process, obviates these tedious Taylor expansions and, using a method of quadratures, shows how to derive a matrix equation which gives the Runge-Kutta equations for any order.

As the order of the process increases the number and complexity of the system of equations which define the parameters in equations (2) also increases; and the minimum number of derivative evaluations (or, see equation (1), evaluations of the function $f(x, y)$) required for an exact solution of the Runge-Kutta equations for a given order increases rapidly.² Since the most time consuming computational aspect is the evaluation of the functions in equations (2), approximate solutions which reduce the number of these derivative determinations is desirable if it is not attained through an unacceptable reduction in accuracy.

Shanks [2, 3] has pioneered in making these approximations and gives values for parameters in equations [2] for orders through eight.³ However, since only the numerical values of these constructions are given, informative material on the techniques for obtaining these parameters, the nature of the approximations and errors, etc., has naturally been suppressed. It is for this reason that the detailed analysis is given here for the fifth and sixth-order cases; and the nature of the analysis, as well as the errors entailed, which are shown here, will frequently demonstrate only simpler aspects of the arithmetically more complex higher-order cases.

¹Rosen, J. S.: The Runge-Kutta Equations by Quadrature Methods. To be published.

²The relation between the order and the number of function evaluations, N , is complex; Butcher [7] deals with this problem. Thus, both Shanks [2] and Butcher [4] have shown that the fifth order requires at least six evaluations for an exact solution.

³He also gives some exact solutions; e. g., he gives the parameters in equations [2] with an adequate value of N to constitute a true solution of the Runge-Kutta equations in the classical sense. For the fifth order Luther and Konen [8] and Luther [9] give a number of these classical Runge-Kutta formulas while Cassity [10] considers the general solution for this order.

THE FIFTH-ORDER RUNGE-KUTTA EQUATIONS IN MATRIX FORM

It will be convenient to express the Runge-Kutta equations in a matrix form. In addition to the advantage of compactness in this form, generalizations may more easily be extended to higher orders.

Two basic sets of relations between the parameters in the Runge-Kutta process may be set down.⁴ The first is

$$(\omega_1 \omega_2 \dots \omega_k) \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & \alpha_2 & \alpha_2^2 & \dots & \alpha_2^m \\ 1 & \alpha_3 & \alpha_3^2 & \dots & \alpha_3^m \\ \vdots & & & & \\ 1 & \alpha_N & \alpha_N^2 & \dots & \alpha_N^m \end{pmatrix} = (1 \ 1/2 \ 1/3 \ \dots \ 1/(m+1)) \quad (5)$$

where $(m+1)$ is the order and N is the number of function evaluations shown in equations (2). The first five equations in Table I are given by equation (5) when $m = 4$.

The second set of relations between the parameters in equations (2) is given by

$$\alpha_{i+1} = \beta_{i+1,1} + \beta_{i+1,2} + \dots + \beta_{i+1,i}, \quad i = 1, 2, \dots, (N-1) \quad (6)$$

We will now give another matrix equation which gives the remainder of the Runge-Kutta equations for the fifth order shown in Table I.

⁴ See footnote 1, page 3.

TABLE I. THE RUNGE-KUTTA EQUATIONS OF THE FIFTH ORDER WITH FIVE EVALUATIONS

$\omega_1 + \omega_2 + \omega_3 + \omega_4 + \omega_5$	$= 1$	(1*)
$\omega_2 \alpha_2 + \omega_3 \alpha_3 + \omega_4 \alpha_4 + \omega_5 \alpha_5$	$= \frac{1}{2}$	(2*)
$\omega_2 \alpha_2^2 + \omega_3 \alpha_3^2 + \omega_4 \alpha_4^2 + \omega_5 \alpha_5^2$	$= \frac{1}{3}$	(3*)
$\omega_2 \alpha_2^3 + \omega_3 \alpha_3^3 + \omega_4 \alpha_4^3 + \omega_5 \alpha_5^3$	$= \frac{1}{4}$	(4*)
$\omega_2 \alpha_2^4 + \omega_3 \alpha_3^4 + \omega_4 \alpha_4^4 + \omega_5 \alpha_5^4$	$= \frac{1}{5}$	(5*)
$\omega_3 \beta_{32} \alpha_2 + \omega_4 (\beta_{42} \alpha_2 + \beta_{43} \alpha_3) + \omega_5 (\beta_{52} \alpha_2 + \beta_{53} \alpha_3 + \beta_{54} \alpha_4)$	$= \frac{1}{6}$	(6*)
$\omega_3 \beta_{32} \alpha_2^2 + \omega_4 (\beta_{42} \alpha_2^2 + \beta_{43} \alpha_3^2) + \omega_5 (\beta_{52} \alpha_2^2 + \beta_{53} \alpha_3^2 + \beta_{54} \alpha_4^2)$	$= \frac{1}{12}$	(7*)
$\omega_3 \beta_{32} \alpha_2^3 + \omega_4 (\beta_{42} \alpha_2^3 + \beta_{43} \alpha_3^3) + \omega_5 (\beta_{52} \alpha_2^3 + \beta_{53} \alpha_3^3 + \beta_{54} \alpha_4^3)$	$= \frac{1}{20}$	(8*)
$\omega_3 \beta_{32} \alpha_2 \alpha_3 + \omega_4 (\beta_{42} \alpha_2 + \beta_{43} \alpha_3) \alpha_3 + \omega_5 (\beta_{52} \alpha_2 + \beta_{53} \alpha_3 + \beta_{54} \alpha_4) \alpha_5$	$= \frac{1}{8}$	(9*)
$\omega_3 \beta_{32} \alpha_2^2 \alpha_3 + \omega_4 (\beta_{42} \alpha_2^2 + \beta_{43} \alpha_3^2) \alpha_4 + \omega_5 (\beta_{52} \alpha_2^2 + \beta_{53} \alpha_3^2 + \beta_{54} \alpha_4^2) \alpha_5$	$= \frac{1}{15}$	(10*)
$\omega_3 \beta_{32} \alpha_2 \alpha_3^2 + \omega_4 (\beta_{42} \alpha_2 + \beta_{43} \alpha_3) \alpha_4^2 + \omega_5 (\beta_{52} \alpha_2 + \beta_{53} \alpha_3 + \beta_{54} \alpha_4) \alpha_5^2$	$= \frac{1}{10}$	(11*)
$\omega_3 \beta_{32} \alpha_2^2 + \omega_4 (\beta_{42} \alpha_2 + \beta_{43} \alpha_3)^2 + \omega_5 (\beta_{52} \alpha_2 + \beta_{53} \alpha_3 + \beta_{54} \alpha_4)^2$	$= \frac{1}{20}$	(12*)
$\omega_4 \beta_{32} \beta_{43} \alpha_2 + \omega_5 [\beta_{32} \beta_{53} \alpha_2 + (\beta_{42} \alpha_2 + \beta_{43} \alpha_3) \beta_{54}]$	$= \frac{1}{24}$	(13*)
$\omega_4 \beta_{32} \beta_{43} \alpha_2 (\alpha_3 + \alpha_4) + \omega_5 [\beta_{32} \beta_{53} \alpha_2 (\alpha_3 + \alpha_5) + (\beta_{42} \alpha_2 + \beta_{43} \alpha_3) \beta_{54} (\alpha_4 + \alpha_5)]$	$= \frac{7}{120}$	(14*)
$\omega_4 \beta_{32} \beta_{43} \alpha_2^2 + \omega_5 [\beta_{32} \beta_{53} \alpha_2^2 + (\beta_{42} \alpha_2^2 + \beta_{43} \alpha_3^2) \beta_{54}]$	$= \frac{1}{60}$	(15*)
$\omega_5 \beta_{32} \beta_{43} \beta_{54} \alpha_2$	$= \frac{1}{120}$	(16*)
$\alpha_2 = \beta_{21}$		
$\alpha_3 = \beta_{31} + \beta_{32}$		
$\alpha_4 = \beta_{41} + \beta_{42} + \beta_{43}$		
$\alpha_5 = \beta_{51} + \beta_{52} + \beta_{53} + \beta_{54}$		

Let us define the matrix

$$\Omega = \begin{pmatrix} \omega_3 & \omega_4 & \omega_5 \\ \omega_3 \alpha_3 & \omega_4 \alpha_4 & \omega_5 \alpha_5 \\ \omega_3 \alpha_3^2 & \omega_4 \alpha_4^2 & \omega_5 \alpha_5^2 \\ \omega_3 c_3^{(1)} & \omega_4 c_4^{(1)} & \omega_5 c_5^{(1)} \\ \gamma_3^{(0)} & \gamma_4^{(0)} & \gamma_5^{(0)} \\ \gamma_3^{(0)} \alpha_3 & \gamma_4^{(0)} \alpha_4 & \gamma_5^{(0)} \alpha_5 \\ \gamma_3^{(1)} & \gamma_4^{(1)} & \gamma_5^{(1)} \\ \gamma_4^{(0)} \beta_{43} + \gamma_5^{(0)} \beta_{53} & \gamma_5^{(0)} \beta_{54} & 0 \end{pmatrix} \quad (7)$$

where

$$\begin{pmatrix} \omega_3 \alpha_3^n & \omega_4 \alpha_4^n & \dots & \omega_N \alpha_N^n \end{pmatrix} \begin{pmatrix} \beta_{32} & 0 & 0 & . & . & . & . & . & 0 \\ \beta_{42} & \beta_{43} & 0 & . & . & . & . & . & 0 \\ \beta_{52} & \beta_{53} & \beta_{54} & 0 & . & . & . & . & 0 \\ \vdots & & & & & & & & \vdots \\ \beta_{N2} & \beta_{N3} & \beta_{N4} & \beta_{N5} & \dots & \dots & \beta_{N,N-1} & 0 \end{pmatrix} \quad (8)$$

$$= \begin{pmatrix} \gamma_2^{(n)} & \gamma_3^{(n)} & \dots & \gamma_N^{(n)} \end{pmatrix}, \quad n = 0, 1, \dots$$

and

$$\begin{aligned} c_3^{(j)} &= \beta_{32} \alpha_2^j \\ c_4^{(j)} &= \beta_{42} \alpha_2^j + \beta_{43} \alpha_3^j \\ &\vdots \\ c_N^{(j)} &= \beta_{N2} \alpha_2^j + \beta_{N3} \alpha_3^j + \dots + \beta_{N,N-1} \alpha_{N-1}^j \end{aligned} \quad (9)$$

$$j = 1, 2, \dots, m-1$$

The matrix (7) then becomes

$$\Omega = \begin{pmatrix} \omega_3 & \omega_4 & \omega_5 \\ \omega_3\alpha_3 & \omega_4\alpha_4 & \omega_5\alpha_5 \\ \omega_3\alpha_3^2 & \omega_4\alpha_4^2 & \omega_5\alpha_5^2 \\ \omega_3\beta_{32}\alpha_2 & \omega_4(\beta_{42}\alpha_2 + \beta_{43}\alpha_3) & \omega_5(\beta_{52}\alpha_2 + \beta_{53}\alpha_3 + \beta_{54}\alpha_4) \\ (\omega_4\beta_{43} + \omega_5\beta_{53}) & (\omega_5\beta_{54}) & 0 \\ (\omega_4\beta_{43} + \omega_5\beta_{53})\alpha_3 & (\omega_5\beta_{54})\alpha_4 & 0 \\ (\omega_4\beta_{43}\alpha_4 + \omega_5\beta_{53}\alpha_5) & (\omega_5\beta_{54})\alpha_5 & 0 \\ (\omega_5\beta_{54})\beta_{43} & 0 & 0 \end{pmatrix}. \quad (10)$$

Let us also define the matrix whose elements are given by (9)

$$C = \begin{pmatrix} \beta_{32}\alpha_2 & \beta_{32}\alpha_2^2 & \beta_{32}\alpha_2^3 \\ \beta_{42}\alpha_2 + \beta_{43}\alpha_3 & \beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2 & \beta_{42}\alpha_2^3 + \beta_{43}\alpha_3^3 \\ \beta_{52}\alpha_2 + \beta_{53}\alpha_3 + \beta_{54}\alpha_4 & \beta_{52}\alpha_2^2 + \beta_{53}\alpha_3^2 + \beta_{54}\alpha_4^2 & \beta_{52}\alpha_2^3 + \beta_{53}\alpha_3^3 + \beta_{54}\alpha_4^3 \end{pmatrix}. \quad (11)$$

Then (See footnote 1, page 3),

$$\Omega C = \begin{pmatrix} 1/6 & 1/12 & 1/20 \\ 1/8 & 1/15 & - \\ 1/10 & - & - \\ 1/20 & - & - \\ 1/24 & 1/60 & - \\ 1/40 & - & - \\ 1/30 & - & - \\ 1/120 & - & - \end{pmatrix} \quad (12)$$

will give the equations (6*) through (16*) (except (14*)⁵) in Table I in the following order:⁶

(6*)	(7*)	(8*)	
(9*)	(10*)	-	
(11*)	-	-	
(12*)	-	-	
(13*)	(15*)	-	(13)
(14a*) #	-	-	
(14b*) #	-	-	
(16*)	-	-	

These⁷ together with equations (5) and (6) are the Runge-Kutta equations for the fifth order with $N = 5$. (See footnote 1.)

REDUCTION OF THE RUNGE-KUTTA EQUATIONS BY SUBSTITUTIONS

The solutions of the Runge-Kutta equations are effected by arbitrarily assuming (except for some restrictions which will be noted later) the values of the parameters α_i and with these values solving the first five equations in Table I for ω_i (or, in the more general case, the $(m + 1)$ equations given by (5)). Since this procedure may be universally used for all orders and for either exact or approximate solutions, the special technique which is applicable to this system of equation is outlined in Appendix A.

⁵Equation (14*) is obtained by adding (14a*) and (14b*) (the equations marked # in (13)).

⁶It will be observed that the numbers of the equations in Table I are distinguished by astrisks.

⁷Equations which are not relevant to our process are indicated by dashes in the equation list (13).

With α_1 and ω_1 known, the remaining Runge-Kutta equations (the equations (6) and the equations from the appropriate matrix equation analogous to equation (12)) are then used to solve for β_{ij} . It is, therefore, to be noted that any transformation which converts the latter Runge-Kutta equations into those given by equation (5) is especially valuable, since this reduces the number of equations in the system which determine the parameters.

We will now show how, by some simple substitutions, we can substantially reduce the number of Runge-Kutta equations in Table I.

In the first column of the matrix (11), let us set

$$c_3^{(1)} = \beta_{32}\alpha_2 = \alpha_3^2/2 \quad (14a)$$

$$c_4^{(1)} = \beta_{42}\alpha_2 + \beta_{43}\alpha_3 = \alpha_4^2/2 \quad (14b)$$

$$c_5^{(1)} = \beta_{42}\alpha_2 + \beta_{53}\alpha_3 + \beta_{54}\alpha_4 = \alpha_5^2/2 = 1/2 \quad (14c)$$

It is immediately evident that equations (6*), (9*), (11*), and (12*) in (13) will be transformed respectively into (3*), (4*), (5*) and (5*) by these substitutions, provided $\omega_2 = 0$, so that the former equations may be removed from further consideration.⁸

The display in the equation list (13) will now leave effectively the following equations:

	(7*)	(8*)	
	(10*)	-	
(13*)	(15*)	-	
(14a*)	-	-	
(14b*)	-	-	
(16*)	-	-	

(15)

⁸For higher orders we can also make similar substitutions for the columns in (11); e. g., we can let $c_i^{(2)} = \alpha_i^2/3$ ($i = 3, 4, 5, \dots$) where $c_i^{(2)}$ is defined by equations (9).

Using the notation in matrices (7) and (8), we can write the following equations on the assumption that equation (14) is used in the matrix C (11):

$$\gamma_2^{(0)} \alpha_2^2 + \gamma_3^{(0)} \alpha_3^2 + \gamma_4^{(0)} \alpha_4^2 = 1/12 \quad (7*)$$

$$\gamma_2^{(0)} \alpha_2^3 + \gamma_3^{(0)} \alpha_3^3 + \gamma_4^{(0)} \alpha_4^3 = 1/20 \quad (8*)$$

$$\gamma_2^{(1)} \alpha_2^2 + \gamma_3^{(1)} \alpha_3^2 + \gamma_4^{(1)} \alpha_4^2 = 1/15 \quad (10*)$$

$$\gamma_3^{(0)} \alpha_3^2 + \gamma_4^{(0)} \alpha_4^2 = 1/12 \quad (13*) \quad (16)$$

$$\gamma_3^{(0)} \alpha_3^3 + \gamma_4^{(0)} \alpha_4^3 = 1/20 \quad (14a*)$$

$$\gamma_3^{(1)} \alpha_3^2 + \gamma_4^{(1)} \alpha_4^2 = 1/15 \quad (14b*)$$

Let us now assume, for the fifth-order approximation, that $\gamma_2^{(0)} = 0$ and furthermore, that $\gamma_2^{(1)}$ is approximately zero; or, sufficiently small so that we may neglect it.⁹ It is immediately apparent from equations (16) that each equation can be paired and that another reduction in the number of equations that have to be satisfied has been achieved. Thus equation list (15) may now be replaced by

-	(13*)	(14a*)	
-	(14b*)	-	
(13*)	(15*)	-	
(14a*)	-	-	(17)
(14b*)	-	-	
(16*)	-	-	

Our problem is to determine the parameters β_{ij} from these equations. Something about the nature of the necessary approximations to solve these equations may be obtained from the following analysis.

⁹ It should be observed that the argument presented here should hold for higher orders as the equations (16) will be unchanged except that there will be more terms.

It may readily be verified by inspection that the equations (13*), (14*),¹⁰ (15*) and (16*) may be represented by the matrix equation

$$\begin{pmatrix} | & | & | & | \\ (\alpha_3 + \alpha_4) & (\alpha_3 + \alpha_5) & (\alpha_4 + \alpha_5) & (\alpha_4 + \alpha_5) \\ \alpha_2 & \alpha_2 & \alpha_2 & \alpha_3 \\ 0 & 0 & 0 & \frac{\alpha_2 \beta_{32}}{\alpha_3} \end{pmatrix} \begin{pmatrix} \omega_4 \alpha_2 (\beta_{32} \beta_{43}) \\ \omega_5 \alpha_2 (\beta_{32} \beta_{53}) \\ \omega_5 \alpha_2 (\beta_{42} \beta_{54}) \\ \omega_5 \alpha_3 (\beta_{43} \beta_{54}) \end{pmatrix} = \begin{pmatrix} 1/24 \\ 7/20 \\ 1/60 \\ 1/120 \end{pmatrix} \quad (18)$$

The (4 x 4) matrix in (18) is singular so that the determinant of the homogenous system is zero. Therefore, in order that the system (18) have solutions, the augmented matrix for the non-homogenous system must be of rank three, in which case it may be verified that the following relation must hold

$$(\alpha_3 - \alpha_2) \alpha_3 + \beta_{32} \alpha_2 (5\alpha_2 - 2) = 0 \quad (19)$$

provided the roots α_3 , α_4 , and α_5 are distinct.

Substituting equation (14a) into equation (19), we get

$$\alpha_2 (5 \alpha_3 - 2) = 0, \quad (20)$$

which together with the condition arising from the choice $\omega_2 = 0$ (see (9-A), Appendix A) restricts the choice of α_1 when $\alpha_5 = 1$ and $\omega_2 = 0$.

Neither of the two solutions that satisfy equation (20) is tenable. α_2 cannot be zero, nor $\alpha_3 = 2/5$, since by the condition (11) in Appendix A it is associated with $\alpha_4 = 1$; and we should recall that a repetitive α is excluded.

We cannot, therefore, satisfy equation (20) exactly; but we can get an approximate solution if we make α_2 small. We shall proceed on this supposition.

¹⁰ See footnote 5, page 8.

OTHER TRANSFORMATIONS

We may now impose certain additional conditions on our parameters and obtain further significant reductions in the Runge-Kutta equations. Huta showed [6, p. 204; 5, p. 8] that what is essentially in our notation,

$$\sum_{i=1}^n \omega_i \beta_{ij} = \omega_j (1 - \alpha_j), \quad j = 1, 2, \dots, N; \quad \beta_{ij} = 0, \quad j \geq i,$$

will hold if

$$\gamma_2^{(0)} = 0, \quad \omega_2 = 0 \quad \text{and} \quad \alpha_N = 1; \quad (21)$$

and, therefore, as may be seen by using matrix (8)¹¹

$$\gamma_j^{(0)} = \omega_j (1 - \alpha_j), \quad j = 3, 4, \dots, N. \quad (22)$$

With these relations it is immediately evident with the help of equations (16) that the equations (7*), (8*), (13*) and (14a*) are satisfied; i.e., these equations are converted into differences of equations in equation (5). However, the importance of these transformations lies not only in these simplifications but also in the fact that they give us simple linear relations from which to calculate the β_{ij} in place of the non-linear Runge-Kutta equations. These linear relations are obtained simply by equating the two definitions of $\gamma_j^{(0)}$ — the one given by matrix (8) and the other by equation (22).

A special, but important, example of this is the relation

$$\gamma_{N-1}^{(0)} = \omega_N \beta_{N,N-1} \quad (23)$$

which follows easily from the definition in matrix (8); but it must be noted it

¹¹See Appendix D for establishing the validity of these transformations.

holds only in this simple form for the (N-N) case. Combining now the two evaluations for $\gamma_{N-1}^{(0)}$ given by equations (22) and (23), we get

$$\gamma_{N-1}^{(0)} = \omega_N \beta_{N,N-1} = \omega_{N-1} (1 - \alpha_{N-1}) \quad . \quad (24)$$

This is an important relation as it immediately gives us one of the parameters $\beta_{N, N-1}$.

THE PARAMETERS FOR THE N^{TH} ORDER WITH N EVALUATIONS

It might be well now to examine the number of equations that are available for finding approximate Runge-Kutta solutions for some of the higher orders. The number of parameters β_{ij} ($j \neq 1$)¹² for the (N-N) Runge-Kutta process can readily be seen from equations (2) to be equal to $(N-1)(N-2)/2$. The number of equations available for finding these parameters are shown in Table II. When the number of available equations (given in the last column of the table) is less than the number of parameters β_{ij} to be found, we can make up this deficiency by using some of the Runge-Kutta equations.

George C. Marshall Space Flight Center
National Aeronautics and Space Administrations
Huntsville, Alabama, April 10, 1967
039-00-24-00-00

¹²When $j = 1$, β_{ij} can be found by using equation (6) after the other β 's have been calculated.

14 TABLE II. THE NUMBER OF EQUATIONS AVAILABLE FOR FINDING THE PARAMETERS β_{ij} ($j \neq 1$)

Order,	No of Parameters β_{ij} ($j \neq 1$) Required $= (N-1) (N-2) / 2$	$c_i^{(1)} = \alpha_i^2 / 2$ is (N-2)	Number of equations available from:			
			$c_i^{(2)} = \alpha_i^3 / 3$ is (N-2)*	(21) and (22) is (N-2)	$\gamma_2^{(1)} = 0$	Total Available Eqs.
5	6	3	0	3	0**	6
6	10	4	0	4	1	9
7	15	5	0	5	1	11
8	21	6	6	6	1	19
9	28	7	7	7	1	22

* When used

** $\gamma_2^{(1)}$ is assumed to be approximately zero in this case.

APPENDIX A

THE WEIGHTS ω_i IN TERMS OF α_i

The weights ω_i in equation (5) can be found in terms of α_i by an effectively simple method [11]. Though the method is general we shall demonstrate this technique for the fifth-order cases with five evaluations.¹

Construct the polynomial

$$\begin{aligned} F(\alpha) &= (\alpha - \alpha_1) (\alpha - \alpha_2) \dots (\alpha - \alpha_5) \\ &= \alpha^5 + a_1\alpha^4 + a_2\alpha^3 + a_3\alpha^2 + a_4\alpha + a_5 \end{aligned} \quad (1-A)$$

where the α_i are parameters in our system of equations ($\alpha_1 = 0$).

We can then construct a second polynomial

$$G(\alpha) = g_4\alpha^4 + g_3\alpha^3 + g_2\alpha^2 + g_1\alpha + g_0 \quad (2-A)$$

whose coefficients are easily determined from the coefficients in equation (1) and the right hand members in the matrix (5). Then, the weights in the system of equations in matrix (5) are given by [11].

$$\omega_i = \frac{G(\alpha_i)}{F'(\alpha_i)}, \quad i = 1, 2, 3, 4, 5. \quad (3-A)$$

We shall limit ourselves for the present to the particular set of solutions where $\alpha_5 = 1$ and $\omega_2 = 0$, so that all subsequent formulas are specialized to these values. We should also note that, although α_1 does not explicitly occur in the Runge-Kutta equations, since it is equal to zero, it does appear in polynomials (1-A) and (3-A).

¹This is the case where $N = m + 1$ in matrix (5). If, as is usually the case, $N > m + 1$ we can revert to the foregoing case by selecting $N - (m + 1)$ values of ω_i .

Hence, when $\alpha_1 = 0$ and $\alpha_5 = 1$, (1-A) takes the special form

$$F(\alpha) = \alpha^5 + a_1\alpha^4 + a_2\alpha^3 + a_3\alpha^2 - (1 + a_1 + a_2 + a_3)\alpha \quad (4-A)$$

where, since the coefficients in (3-A) are the symmetric functions involving its roots,

$$a_1 = -(\alpha_2 + \alpha_3 + \alpha_4 + 1)$$

$$a_2 = (\alpha_2\alpha_3 + \alpha_2\alpha_4 + \alpha_3\alpha_4) + (\alpha_2 + \alpha_3 + \alpha_4) \quad (5-A)$$

$$a_3 = -\alpha_2\alpha_3\alpha_4 - (\alpha_2\alpha_3 + \alpha_2\alpha_4 + \alpha_3\alpha_4)$$

while the coefficients of $G(\alpha)$ in (2-A) are given by [11]

$$g_4 = 1$$

$$g_3 = a_1 + 1/2$$

$$g_2 = a_2 + (1/2)a_1 + 1/3 \quad (6-A)$$

$$g_1 = a_3 + (1/2)a_2 + (1/3)a_1 + 1/4$$

$$g_0 = (-1/2)a_3 - (2/3)a_2 - (3/4)a_1 - 4/5 \quad .$$

We shall also find useful the cubic derived from equation (4-A)

$$f(\alpha) = \alpha^3 + (a_1 + 1)\alpha^2 + (a_2 + a_1 + 1)\alpha + (a_3 + a_2 + a_1 + 1) = 0 \quad (7-A)$$

which has the roots α_2 , α_3 and α_4 .

The Condition For $\omega_2 = 0$

Since we are assuming that $\omega_2 = 0$, an important condition may be derived when we note from equation (3-A) that $G(\alpha_2) = 0$ must hold, provided $F'(\alpha_2) \neq 0$. However, we can exclude $F'(\alpha_2) = 0$, since this would denote a double root α_2 in $F(\alpha)$. We can expedite the determination of this condition if we evaluate instead

$$2G(\alpha_2) - (2\alpha_2 + 1) f(\alpha_2) = 0 \quad (8-A)$$

since by equation (7-A) α_2 is also a root of $f(\alpha) = 0$.

After somewhat tedious algebraic operations on substituting the a 's given in equation (5-A) into equation (8-A), we get

$$10\alpha_3\alpha_4 - 5(\alpha_3 + \alpha_4) + 3 = 0. \quad (9-A)$$

This is a relation that must subsist between the two parameters when $\omega_2 = 0$, $\alpha_1 = 0$ and $\alpha_5 = 1$.

Formulae For The Weights ω_i

Since $G(\alpha_2) = 0$, we can write equation (3-A) in the form

$$\omega_i = \frac{(\alpha_i - \alpha_2) h(\alpha_i)}{F'(\alpha_i)}, \quad i = 1, 2, 3, 4, 5 \quad (10-A)$$

where, by dividing $G(\alpha)$ synthetically by $(\alpha - \alpha_2)$, or factoring by other means, we find

$$h(\alpha) = \alpha^3 + h_1\alpha^2 + h_2\alpha + h_3 \quad (11-A)$$

where

$$\begin{aligned}
 h_1 &= \alpha_2 + g_3 = -(\alpha_3 + \alpha_4 + 1/2) \\
 h_2 &= h_1\alpha_2 + g_2 = \alpha_3\alpha_4 + (1/2)(\alpha_3 + \alpha_4) - 1/6 \\
 h_3 &= h_2\alpha_2 + g_1 = -\alpha_2\alpha_3\alpha_4 - (1/2)(\alpha_2\alpha_3 + \alpha_2\alpha_4 + \alpha_3\alpha_4) \\
 &\quad + (1/6)(\alpha_2 + \alpha_3 + \alpha_4) - 1/12 .
 \end{aligned} \tag{12-A}$$

Using equation (9-A), these may be simplified so that we get

$$\begin{aligned}
 h(\alpha) &= \alpha^3 - (\alpha_3 + \alpha_4 + 1/2)\alpha^2 + (\alpha_3 + \alpha_4 - 7/15)\alpha \\
 &\quad - (1/60)[5(\alpha_3 + \alpha_4) - 4] .
 \end{aligned} \tag{13-A}$$

It will be observed that the coefficients of $h(\alpha)$ in equation (13-A) are independent of α_2 .

With the aid of the first equation in (1-A) we can readily find the $F'(\alpha_i)$.

These are:

$$\begin{aligned}
 F'(\alpha_1) &= \alpha_2\alpha_3\alpha_4, & \alpha_1 &= 0 \\
 F'(\alpha_2) &= \alpha_2(\alpha_2 - \alpha_3)(\alpha_2 - \alpha_4)(\alpha_2 - 1), \\
 F'(\alpha_3) &= \alpha_3(\alpha_3 - \alpha_2)(\alpha_3 - \alpha_4)(\alpha_3 - 1), \\
 F'(\alpha_4) &= \alpha_4(\alpha_4 - \alpha_2)(\alpha_4 - \alpha_3)(\alpha_4 - 1), \\
 F'(\alpha_5) &= \alpha_5(\alpha_5 - \alpha_2)(\alpha_5 - \alpha_3)(\alpha_5 - \alpha_4) \\
 &= (1 - \alpha_2)(1 - \alpha_3)(1 - \alpha_4), & \alpha_5 &= 1 .
 \end{aligned} \tag{14-A}$$

Using these in (10-A), the formulae for the weights, we get

$$\omega_1 = -h(0)/\alpha_3\alpha_4 \tag{15-A}$$

$$\omega_2 = 0 \quad (16-A)$$

$$\omega_3 = h(\alpha_3) / \alpha_3(\alpha_3 - \alpha_4) (\alpha_3 - 1) \quad (17-A)$$

$$\omega_4 = h(\alpha_4) / \alpha_4(\alpha_4 - \alpha_3) (\alpha_4 - 1) \quad (18-A)$$

$$\omega_5 = h(\alpha_5) / (\alpha_3 - 1) (\alpha_4 - 1) \quad , \quad \alpha_5 = 1 \quad (19-A)$$

It should be observed that, in view of our previous observation on the coefficients of $h(\alpha)$ in equation (13-A), the ω_i also are independent of α_2 .

An Alternate Method

An alternate method (which we will find useful to refer to later) is to solve the linear system of equations (5) by determinants. We will illustrate this for the sixth-order case ($N = 6$, $m = 5$) as our method may easily be extended to higher orders.

For ω_2 we have the ratio of the two determinants:

$$\begin{vmatrix} | & | & | & | & | & | \\ 0 & 1/2 & \alpha_3 & \alpha_4 & \alpha_5 & \alpha_6 \\ 0 & 1/3 & \alpha_3^2 & \alpha_4^2 & \alpha_5^2 & \alpha_6^2 \\ 0 & 1/4 & \alpha_3^3 & \alpha_4^3 & \alpha_5^3 & \alpha_6^3 \\ 0 & 1/5 & \alpha_3^4 & \alpha_4^4 & \alpha_5^4 & \alpha_6^4 \\ 0 & 1/6 & \alpha_3^5 & \alpha_4^5 & \alpha_5^5 & \alpha_6^5 \end{vmatrix} \quad (20-A)$$

and

$$\begin{vmatrix}
 0 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 & \alpha_6 \\
 0 & \alpha_2^2 & \alpha_3^2 & \alpha_4^2 & \alpha_5^2 & \alpha_6^2 \\
 0 & \alpha_2^3 & \alpha_3^3 & \alpha_4^3 & \alpha_5^3 & \alpha_6^3 \\
 0 & \alpha_2^4 & \alpha_3^4 & \alpha_4^4 & \alpha_5^4 & \alpha_6^4 \\
 0 & \alpha_2^5 & \alpha_3^5 & \alpha_4^5 & \alpha_5^5 & \alpha_6^5
 \end{vmatrix} \quad (21-A)$$

These determinants may be further simplified for we can reduce the order of determinants (20-A) and (21-A) by taking the cofactor of 1 in the first column. Then if we set $\alpha_6 = 1$ and subtract adjacent rows, we get for determinant (20-A)

$$\begin{vmatrix}
 1/6 & \alpha_3(1-\alpha_3) & \alpha_4(1-\alpha_4) & \alpha_5(1-\alpha_5) & 0 \\
 1/12 & \alpha_3^2(1-\alpha_3) & \alpha_4^2(1-\alpha_4) & \alpha_5^2(1-\alpha_5) & 0 \\
 1/20 & \alpha_3^3(1-\alpha_3) & \alpha_4^3(1-\alpha_4) & \alpha_5^3(1-\alpha_5) & 0 \\
 1/30 & \alpha_3^4(1-\alpha_3) & \alpha_4^4(1-\alpha_4) & \alpha_5^4(1-\alpha_5) & 0 \\
 1/6 & \alpha_3^5 & \alpha_4^5 & \alpha_5^5 & 1
 \end{vmatrix} \quad (22-A)$$

which reduces to

$$(1-\alpha_3) (1-\alpha_4) (1-\alpha_5) \begin{vmatrix}
 1/16 & \alpha_3 & \alpha_4 & \alpha_5 \\
 1/12 & \alpha_3^2 & \alpha_4^2 & \alpha_5^2 \\
 1/20 & \alpha_3^3 & \alpha_4^3 & \alpha_5^3 \\
 1/30 & \alpha_3^4 & \alpha_4^4 & \alpha_5^4
 \end{vmatrix} \quad (23-A)$$

Similarly determinant (21-A) can be reduced to

$$(1-\alpha_2) (1-\alpha_3) (1-\alpha_4) (1-\alpha_5) \begin{vmatrix} \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 \\ \alpha_2^2 & \alpha_3^2 & \alpha_4^2 & \alpha_5^2 \\ \alpha_2^3 & \alpha_3^3 & \alpha_4^3 & \alpha_5^3 \\ \alpha_2^4 & \alpha_3^4 & \alpha_4^4 & \alpha_5^4 \end{vmatrix} \quad (24-A)$$

so that $\omega_2 (1-\alpha_2)$ is given by the ratio of the determinants in (23-A) and (24-A):

$$\begin{vmatrix} 1/16 & \alpha_3 & \alpha_4 & \alpha_5 \\ 1/12 & \alpha_3^2 & \alpha_4^2 & \alpha_5^2 \\ 1/20 & \alpha_3^3 & \alpha_4^3 & \alpha_5^3 \\ 1/30 & \alpha_3^4 & \alpha_4^4 & \alpha_5^4 \end{vmatrix} \div \begin{vmatrix} \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 \\ \alpha_2^2 & \alpha_3^2 & \alpha_4^2 & \alpha_5^2 \\ \alpha_2^3 & \alpha_3^3 & \alpha_4^3 & \alpha_5^3 \\ \alpha_2^4 & \alpha_3^4 & \alpha_4^4 & \alpha_5^4 \end{vmatrix} \quad (25-A)$$

Similar ratios may be found for the expressions $\omega_i (1 - \alpha_i)$.

It is evident that the vanishing of the determinant (23-A) is a condition for $\omega_2 = 0$ provided $\alpha_6 = 1$ and $\alpha_i \neq 1$ ($i = 3, 4, 5$).²

²To obtain this condition for the fifth-order case delete the last row and column in the determinant (21-A) and set $\alpha_5 = 1$. The vanishing of this determinant is the relation (9).

APPENDIX B

THE PARAMETERS FOR THE FIFTH ORDER WITH FIVE EVALUATIONS

We shall now show how the six parameters β_{ij} ($j \neq 1$)¹ for the approximate fifth-order Runge-Kutta process with five evaluations may be found. We assume that the values of α_3 and α_4 have been selected (subjected to the condition (9-A)) and that the ω 's have been obtained as indicated in Appendix A. We can now proceed as follows -- expressing the parameters in terms of the known α_3 , α_4 and ω_1 :²

- 1) Calculate β_{32} by equation (14a):

$$\beta_{32} = \alpha_3^2 / 2\alpha_2 \quad .$$

- 2) Calculate β_{54} by using equation (24) which defines $\gamma_4^{(0)}$ in two ways:

$$\gamma_4^{(0)} = \omega_5 \beta_{54} = \omega_4 (1 - \alpha_4) \quad ,$$

so that

$$\beta_{54} = \omega_4 (1 - \alpha_4) / \omega_5 \quad .$$

- 3) Calculate β_{43} using equation (16*):

$$\beta_{43} = \frac{1}{60 \omega_5 \alpha_3^2 \beta_{54}} = \frac{1}{60 \alpha_3^2 \omega_4 (1 - \alpha_4)} \quad .$$

¹When $j = 1$, β_{ij} can be found by using equation (6) after the other β 's have been calculated.

²As previously observed the ω_i are independent of α_2 so that in the subsequent results α_2 is a free parameter.

4) Calculate β_{42} using equation (14b):

$$\beta_{42} = \frac{1}{\alpha_2} \left(\frac{\alpha_4^2}{2} - \beta_{43}\alpha_3 \right) .$$

5) Calculate β_{52} using $\gamma_2^{(0)} = 0$:

$$\beta_{52} = -\frac{1}{\omega_5} (\omega_3\beta_{32} + \omega_4\beta_{42}) .$$

6) Calculate β_{53} using equation (14c):

$$\beta_{53}\alpha_3 = \frac{1}{2} - (\beta_{52}\alpha_2 + \beta_{54}\alpha_4)$$

or, instead use

$$\gamma_3^{(0)} = \omega_4\beta_{43} + \omega_5\beta_{53} = \omega_3(1-\alpha_3)$$

the two results should check.

APPENDIX C

THE SIXTH-ORDER RUNGE-KUTTA APPROXIMATION WITH SIX EVALUATIONS

We shall outline a step-by-step procedure for obtaining the parameters for the sixth-order Runge-Kutta approximation with six evaluations.

As outlined in Appendix B for the fifth-order case, we can in a similar way select values for α_i (with some restrictions) and find the ω_i . As we assume equations (21) to hold, it is true that $\alpha_6 = 1$ and $\omega_2 = 0$; and it is this last relation which dictates a condition between the α_i ($i = 3, 4, 5$) analogous to (9-A), and which we will not stop to derive.

As we may see from Table II we can assume that the following hold: the four relations analogous to equation (14);¹ the four relations in equations (21) and (22); and finally, that $\gamma_2^{(1)} = 0$;² a total of nine relations for ten unknown parameters. We are thus free to make use of another Runge-Kutta equation; and we might make use of the equation analogous to equation (16*) which was found useful in the fifth-order case. This is:³

$$\omega_6 \beta_{32} \beta_{43} \beta_{54} \beta_{65} \alpha_2 = \frac{1}{6!} \quad (1-C)$$

We now proceed as follows:

- 1) Calculate β_{32} using equation (14a):

$$\beta_{32} = \alpha_3^2 / 2\alpha_2 \quad (2-C)$$

$$^1 C_i^{(1)} = \alpha_i^2 / 2 \quad (i = 3, 4, 5, 6).$$

²See footnote 9. Since the equations in (16) will hold for the sixth-order case also (except for additional terms), it may be seen that in this group (10*) would revert to equation (14b*) if we set $\gamma_2^{(1)} = 0$. This assumption is vital to the simplifications necessary to reduce the complexity of the computations given here.

³See footnote 1, page 3.

2) Using the relations $\gamma_5^{(0)} = \omega_6 \beta_{65} = \omega_5 (1 - \alpha_5)$ given by equation (24) :

$$\beta_{65} = \omega_5 (1 - \alpha_5) / \omega_6 \quad . \quad (3-C)$$

(The subsequent β 's are all calculated in terms of the unknown β_{54} .)

3) Using equation (1-C) calculate β_{43} :

$$\beta_{43} = \left(\frac{2}{6! \omega_6 \beta_{65} \alpha_3^2} \right) \frac{1}{\beta_{54}} \quad . \quad (4-C)$$

4) Calculate β_{42} using equation (14b) :

$$\beta_{42} = \frac{1}{\alpha_2} \left[\frac{\alpha_4^2}{2} - \beta_{43} \alpha_3 \right] \quad . \quad (5-C)$$

5) Solve for β_{52} using the relations:

$$\begin{aligned} \gamma_2^{(0)} &= \omega_3 \beta_{32} + \omega_4 \beta_{42} + \omega_5 \beta_{52} + \omega_6 \beta_{62} = 0 \\ \gamma_2^{(1)} &= \omega_3 \beta_{32} \alpha_3 + \omega_4 \beta_{42} \alpha_4 + \omega_5 \beta_{52} \alpha_5 + \omega_6 \beta_{62} \alpha_6 = 0 \end{aligned} \quad (6-C)$$

which by subtraction gives (Since $\alpha_6 = 1$)

$$\gamma_2^{(0)} - \gamma_2^{(1)} = \omega_3 (1 - \alpha_3) \beta_{32} + \omega_4 (1 - \alpha_4) \beta_{42} + \omega_5 (1 - \alpha_5) \beta_{52} = 0 \quad . \quad (7-C)$$

6) Solve (in terms of β_{54}) for β_{53} using

$$c_5^{(1)} = \beta_{52} \alpha_2 + \beta_{53} \alpha_3 + \beta_{54} \alpha_4 = \alpha_5^2 / 2 \quad (8-C)$$

7) Substitute the foregoing values of β_{ij} into equations (21) and (22) where $\gamma_2^{(0)}$, $\gamma_3^{(0)}$ and $\gamma_4^{(0)}$ are expanded by equations (8) and find β_{62} , β_{63} and β_{64} in terms of β_{54} .

8) Finally determine β_{54} by substituting the above values of β_{ij} into

$$c_6^{(1)} = \beta_{62}\alpha_2 + \beta_{63}\alpha_3 + \beta_{64}\alpha_4 + \beta_{65}\alpha_5 = \alpha_6^2/2 = 1/2 \quad . \quad (9-C)$$

APPENDIX D

THE VALIDITY OF THE TRANSFORMATION $\gamma_i^{(0)} = \omega_i (1 - \alpha_i)$

It would be desirable to examine the validity of assuming equations (21) and (22) when seeking approximate Runge-Kutta solutions. We will illustrate this with an analysis for the sixth-order case with six evaluations as the procedure can easily be adapted to higher order cases.

Let us examine the effect of these transformations on the linear system analogous to (6*), (7*) and (8*) -- the equations in the first row in the equation list (13). (See also equations (16).) For the sixth-order there will be an additional equation in the system and each equation will have an additional term; these will be given by (see footnote 1 page 3 , Table I)

$$\gamma_2^{(0)} \alpha_2^n + \gamma_3^{(0)} \alpha_3^n + \gamma_4^{(0)} \alpha_4^n + \gamma_5^{(0)} \alpha_5^n = 1/(n+1) (n+2) \quad (1-D)$$

$$n = 1, 2, 3, 4 \quad .$$

It is immediately evident that the substitutions of equations (21) and (22) into the system (1-D) gives us simple combinations of equations in system (5) if $\alpha_6 = 1$, so that the advantage of these substitutions is apparent. However, we must see if equations (21) and (22) are acceptable as solutions of the system (1-D).

If we solve the linear system (1-D) for $\gamma_2^{(0)}$ using determinants, we get

$$\begin{vmatrix} 1/6 & \alpha_3 & \alpha_4 & \alpha_5 \\ 1/12 & \alpha_3^2 & \alpha_4^2 & \alpha_5^2 \\ 1/20 & \alpha_3^3 & \alpha_4^3 & \alpha_5^3 \\ 1/30 & \alpha_3^4 & \alpha_4^4 & \alpha_5^4 \end{vmatrix} \div \begin{vmatrix} \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 \\ \alpha_2^2 & \alpha_3^2 & \alpha_4^2 & \alpha_5^2 \\ \alpha_2^3 & \alpha_3^3 & \alpha_4^3 & \alpha_5^3 \\ \alpha_2^4 & \alpha_3^4 & \alpha_4^4 & \alpha_5^4 \end{vmatrix} \quad (2-D)$$

which we have shown in equation (25-A) to be $\omega_2(1-\alpha_2)$.

In the same way we can quite readily justify the other transformations in equation (22).

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